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Decisions on air quality problems must often be made on the basis of existing ambient air quality data. One consideration in such situations is how to accomodate the uncertainty associated with these measurements. Measurement error is often stated in terms of a single measurement, while the decision is made on the basis of the entire data set for a year. Therefore, there is a practical need to translate the uncertainty statement for a single measurement into an uncertainty statement for the decision-making statistic. In a sense, the quality assurance statement for an individual measurement should be transformed into a quality assurance statement that is applicable to the decision that is made from the data. This paper develops an empirical Bayes framework for this type of problem and examines the application of this technique for a short-term National Ambient Air Quality Standard. The analytical results obtained from the empirical Bayes methodology are compared to results obtained from computer simulations.

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Decisions on air quality problems must often be made on the basis of existing ambient air quality data. One consideration in such situations is how to accomodate the uncertainty associated with these measurements. Measurement error is often stated in terms of a single measurement, while the decision is made on the basis of the entire data set for a year. Therefore, there is a practical need to translate the uncertainty statement for a single measurement into an uncertainty statement for the decision-making statistic. In a sense, the quality assurance statement for an individual measurement should be transformed into a quality assurance statement that is applicable to the decision that is made from the data. This paper develops an empirical Bayes framework for this type of problem and examines the application of this technique for a short-term National Ambient Air Quality Standard. The analytical results obtained from the empirical Bayes methodology are compared to results obtained from computer simulations.

Introduction

Measurement uncertainty must be recognized as a fact of life in any existing air pollution monitoring network. This is not because of any lack of interest in improving the quality of ambient air pollution measurements but is simply due to the practical constraints and limitations of current air pollution measurement technology. The purpose of this paper is to examine an alternative data analysis technique that could be used to enhance the quality of the information obtained from the available ambient data base. In particular, this paper focuses upon the use of a Bayesian statistical framework to account for the effect of measurement uncertainty in problems relating to attainment/nonattainment classification.

Air pollution measurement uncertainty is frequently described in terms of the uncertainty associated with an individual measurement. While this is obviously of interest, decisions are typically made on the basis of a larger data set consisting of a year or more of data. Therefore, it is necessary to translate the uncertainty statement for an individual measurement into an uncertainty statement that is applicable to the decision-making value that is obtained from the entire data set. Some aspects of this problem have been examined by employing computer simulations [1]. It was found that unbiased individual measurements could result in biased peak value summary statistics. These results lend further credence to the viewpoint that a methodology is needed to develop uncertainty statements that are directly related to the decision that must be made.

A practical problem where this type of information could be useful is in attainment/nonattainment classification. For example, the present National Ambient Air Quality Standard (NAAQS) for total suspended particulate (TSP) specifies that no more than one 24-hr measurement per year should exceed 260 $\mu g/m^3$ [2]. Therefore, while the uncertainty associated with an individual measurement is of interest, it would also be desirable to be able to make a probability statement concerning the likelihood that a particular site is nonattainment based upon all of the available data for the year and the measurement uncertainty of the individual measurements.

One possible approach to this type of problem is the use of the empirical Bayes statistical framework. This approach was used previously by Suggs and Curran [3] to incorporate individual measurement uncertainty into a probability statement that a specific measurement exceeded the level of the standard. This present paper examines the possibility of extending this approach to consider all of the available data. A methodology that considers all of the data avoids the potential bias of only focusing on the measurement error for values that are above the level of the standard and ignoring the possibility that there are two sides to the problem; a measurement above the standard may be artifically high due to measurement error, but at the same time a measurement may be too low due to measurement error. This extension considered here may be viewed intuitively as a two-step process. In the first step, the previous methodology is applied to each measurement to determine the probability that that particular measurement is above the level of the standard. For convenience, this is termed an "exceedance probability." In the second step, these individual exceedance probabilities can then be used to compute the expected number of exceedances for a year. Alternatively these individual exceedance probabilities could be used to calculate the probability of a violation, i.e., that two or more measurements in the year were above the level of the standard.

The following sections present a formal development of the statistical methodology, examples illustrating how the technique could be employed, and then a brief discussion of the interpretation of the results.

Development of the Method

Although measurement uncertainty is an inherent influence in determining exceedances, it currently plays no explicit role in air quality evaluations. However, it might be possible to incorporate measurement uncertainty into existing decision making processes in a way that broadens the scope of current practices of determining attainment status. For example, a single 24-h measurement, X_i (i=1, 2...n), is used to determine if the true TSP concentration, μ_i, is below the standard level of 260 $\mu g/m^3$ for the i^{th} day. Without considering measurement uncertainty in a probabilistic framework, there is no mechanism for judging if an exceedance is real or possibly attributable simply to random variation alone. From the viewpoint of the data user, the question of interest may be stated by asking how likely it is that the observed measurement reflects a value that is truly greater than the level of the standard. [This question differs from the more common statistical framework which would examine the likely distribution of the measured value for an assumed true value.] If we consider that the true concentrations can be treated as random variables with a probability distribution denoted by P(U), we can use Bayesian statistics to determine the conditional probability, $P_i(H|X_i)$, where $H:\mu_i>260$, that the true concentration level exceeds the standard level for the i^{th} unit of time given X_i. The distribution P(U) is referred to as the "prior" and $P_i(H|X_i)$ is referred to as the "posterior" distribution in Bayesian terminology. Each posterior (or exceedance) probability is calculated with the aid of Bayes formula [4]:

$$P_i(H|X_i) = \frac{P(U)P(X|\mu_i)}{P(X)}. \qquad (1)$$

The above expression basically states that the probability of $H:\mu>260\mu g/m^3$ given X_i, is proportional to the prior distribution, P(U), times the likelihood function of the measurement. Under certain assumptions commonly associated with air pollution measurements [3], the posterior distribution is described as being normally distributed with mean

$$\alpha = \frac{\theta T^2 + \log X_i \beta^2}{T^2 + \beta^2} \qquad (2)$$

and variance

$$\gamma^2 = \frac{T^2\beta^2}{T^2 + \beta^2} \qquad (3)$$

where

$$\theta = \frac{\sum_{i=1}^{n} \log X_i}{n} \qquad (4)$$

and

$$\beta^2 = \frac{\sum_{i=1}^{n} (\log X_i - \theta)^2 - T^2}{n-1} \qquad (5)$$

are parameter estimates of the prior distribution and T is the measurement imprecision expressed as a per cent coefficient of variation. Replacing precise knowledge with empirical estimates from equations 4 and 5 and the assumption that a prior distribution exists but may be unknown is a less strict but more practical approach referred to as "empirical Bayes" [5].

The basic statistical model providing the foundation for this approach is:

$$X_i = \mu_i + \varepsilon_i \tag{6}$$

where X_i = measured value for the i^{th} unit of time
μ_i = true value for the i^{th} unit of time
ε_i = imprecision of the i^{th} measurement.

All variables in the model are assumed random with no fixed bias since bias is considered a less serious error that can effectively be controlled with calibration procedures. The assumption of randomness seems reasonable since true concentrations are the products of emissions and atmospheric conditions that combine in a time-varying way that is not totally predictable. We will also assume that the true concentrations are lognormally distributed

$$\text{e.g.,} \quad \log(U) \sim N(\theta, \beta^2).$$

Measurement imprecision is considered to be normally distributed with a standard deviation, σ_i, proportional to the true value. Therefore, the model can be rewritten as

$$\begin{aligned} X_i &= \mu_i (1 + \varepsilon_i/\mu_i) \\ &= \mu_i \delta_i \end{aligned} \tag{7}$$

It follows that

$$\log X_i = \log \mu_i + \log \delta_i \tag{8}$$

where $\log(\delta_i) \sim N(0, T^2)$

as long as the coefficient of variation $T = \sigma_i/\mu_i$ is less than 1/3 [6]. It should also be noted that the variable X is lognormally distributed with mean θ and variance $\beta^2 + T^2$.

The potential application of this posterior disbribution to attainment/nonattainment decisions was discussed to some extent in a paper by Suggs and Curran [3]. For example, if a site has a history of high TSP concentrations as indicated by a geometric mean of 112.7 $\mu g/m^3$ and a geometric standard deviation of 1.62 $\mu g/m^3$, then there is a high probability (.80) that the true concentration exceeds the standard when a measurement of 274 $\mu g/m^3$, (just 5% higher than the standard) is taken with a measurement imprecision of 5% coefficient of variation. Table 1 presents the probability that a measured value of 274 $\mu g/m^3$ would represent a true exceedance for various levels of measurement imprecision. The results coincide with the intuitive idea that, as the level of measurement imprecision increases, there is less confidence that the value represents a true exceedance. [It should be noted that the probabilities in this Table are affected by the distributional approximation and should be viewed as directionally correct although the absolute magnitude, particularly for the higher levels of imprecision, is affected by this approximation.][7]

TABLE 1. EXCEEDANCE PROBABILITIES FOR SEVERAL VALUES OF T WHEN X = 274 $\mu g/m^3$

T(%)	Prob(μ>260 | X = 274)
5	.81
10	.56
15	.40
20	.29
25	.19
30	.10

Using the Bayesian estimate of probability to incorporate measurement imprecision broadens the information involved in determining attainment status. The basis of a decision would involve three considerations: (1) current measurements, (2) past history, and (3) a probability level. It is interesting to note that if the yearly geometric mean had been 56.65 $\mu g/m^3$ (well below the NAAQS for a TSP yearly mean), then the probability of a true exceedance is reduced to 0.74 for a measurement of 274 $\mu g/m^3$ with a 5% coefficient of variation. The Bayesian estimate basically states that the "high values are more plausible when they are supported by previous data than when they represent a departure from previous patterns" [3]. This methodology can easily be expanded to incorporate measurement imprecision and historical data into calculating exceedance rates, as discussed in the next paragraph.

Given a set of measurements $\{X_1, X_2 \ldots . X_n\}$, we can calculate a set of probabilities $\{P_i(H|X_i) \ldots . P_n(H|X_n)\}$ and compute the probability of a violation (i.e., two or more exceedances) which would be applicable to old style standards. Or we could compute the expected number of exceedances for the entire time period by summing the posterior probabilities over all measurements; that is

$$N_E = \sum_{i=1}^{n} P_i(H|X_i). \tag{9}$$

It should be noted that to determine the probability of a violation involves the actual X_i sequence along with the assumption of independence in the observations to make the calculation statistically more tractable. This assumption is not required for determining the expected number of exceedances. According to the following calculation of the expected number of exceedances using the Bayesian estimate:

$$E(N_E) = E\left(\sum_{i=1}^{n} P_i(H|Xi)\right) \tag{10}$$

$$= \sum_{i=1}^{n} E(P_i(H|X_i))$$

$$= \sum_{i=1}^{n} \int P_i(H|X_i)P(X_i)dX_i$$

$$= \sum_{i=1}^{n} \int P(H|X)P(X)dX$$

$$= n * P(H), \tag{11}$$

the Bayesian estimate is proportional to the total sample size n by an amount equal to the marginal distribution of X. In other words, the Bayesian estimate of exceedance rates is independent of measurement imprecision with an expected value equal to the exceedance rate of the prior distribution of true values.

According to Curran [1] measurement imprecision creates an overestimate in the number of peak values. The Bayesian procedure adjusts for any overestimations that may be attributed to random fluctuations. This provides an attainment test that pertains to the true values. If an exceedance rate goes beyond that specified by the standard for a site that has historically

been attainment, it is more likely that a real exceedance has occurred rather than something that can be attributed to random fluctuations alone.

Application of the Method

To demonstrate how this methodology can be applied, a computer simulation was used to create and sample from populations that on the average contain only one exceedance per year for TSP. These populations are characterized by three geometric standard deviations: 1.2, 1.6, and 2.0 There are other acceptable combinations of means and standard deviations for lognormal distributions with a characteristic high of 260 $\mu g/m^3$, but the ones chosen here represent a fairly common range. The simulation results are based upon 100 trial years of daily data. The measurement imprecision is set at ± 5%, ± 10%, and ± 15% coefficient of variation. The observed exceedances are tabulated along with the Bayesian estimate for each year and averaged over the 100 years.

The results shown in Table II are consistent with those obtained from other computer simulation studies [1]. Measurement imprecision causes a positive bias in the observed exceedance rate. On the other hand, the Bayesian estimate is more accurate than the observed rate which is also consistent with the theory. Inaccuracies occur for the higher imprecision and are more noticeable when the true distribution has a geometric standard deviation of 1.2 $\mu g/m^3$. The underestimate associated with the Bayesian estimates are attributed to the approximation used to derive the posterior distribution as was previously pointed out in the discussion of Table I. The effects are less noticeable for measurement imprecision of 10% or less for true distributions with relatively more spread (e.g., geometric standard deviation greater than 1.6). In any case, the Bayesian estimates are more accurate than the observed rates.

Discussion

There are some notes of practical interest concerning the application of the Bayesian method to determing exceedance rates. The Bayesian method considers the entire sample, and in most cases can be viewed as a cautious approach requiring more than two measurements above the standard to produce a Bayesian exceedance rate of more than one per year. The effect of measurements far below the standard level are insignificant to the exceedance rate calculation. The Bayesian method also offers an objective approach to dealing with borderline cases. Under the present system, a measurement of 260 $\mu g/m^3$ could conceivably occur several times but no exceedance could be claimed. Using the Bayesian method, several borderline measurements could translate into an expected exceedance greater than 1.0 depending on the prior distribution and the measurement uncertainty.

TABLE II. EXCEEDANCE RATES - OBSERVED/BAYESIAN

		% C.V.			
		0*	5	10	15
geo.std.dev.	1.2	.93	1.22/.88	2.07/.75	4.06/.65
	1.6	1.02	1.03/1.00	1.17/.99	1.37/.92
	2.0	1.03	1.01/1.00	1.04/.98	1.08/.94

*True exceedance rate (i.e., sampling with 0% error)

TABLE III. BAYESIAN EXCEEDANCE ESTIMATES FOR CASES WITH FIVE BORDERLINE EXCEEDANCES

		geo. std. dev.		
		1.2	1.6	2.0
% CV	5	1.02	2.10	2.10
	10	.42	1.35	1.72
	15	.17	1.00	1.35

For example, Table III shows the Bayesian exceedance rate when five TSP measurements of 260 $\mu g/m^3$ are measured with 5, 10, and 15% imprecision. Three different prior distributions are represented each with a characteristic high of 260 $\mu g/m^3$. It seems intuitively objectionable that any site could have so many borderline cases and yet not have at least one exceedance. Summing the exceedance probabilities for only the five borderline measurements resulted in an expected exceedance rate of at least 1.0 for all but the lighter tailed prior with a 1.2 geometric standard deviation and where measurement imprecision was 10% and greater. In each of these cases the borderline values produced an exceedance probability of 0.2 or greater even though the measurements themselves were exactly 260 $\mu g/m^3$.

Conclusions

The example applications considered here illustrate the feasibility of applying the empirical Bayes framework to determining expected exceedance rates for statistical air quality standards and could also be used to compute probabilities for deterministic standards. The results for the simulation studies are intuitively reasonable. However, the statistical approximation used in the mathematical development appears to produce an underestimate in the exceedance rates. This suggest that more theoretical work may be necessary to refine the computations. As part of this extension, consideration should be given to alternative distributional representations of the underlying air quality distributions because it is well known that statistical distributions other than the lognormal frequently offer better characterization of air quality data. Nevertheless, the basic empirical Bayes approach appears to offer a promising framework for eventually incorporating measurement imprecision into air quality decision-making.

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